

Coupled Thermomechanical Micromechanics Modeling of the Influence of Thermally Grown Oxide Layer in an Environmental Barrier Coating System

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Introduction

Aircraft engine efficiency can be significantly improved with advanced materials

- Higher temperature materials require less cooling air
- Lower density materials can lead to lower weight of components

Ceramic Matrix Composites (CMCs) offer a significant improvement over metals

- CMCs with 2400°F capability began flying in commercial aircraft engines in 2016
- This is ~300°F higher temperature capability than metals, at 1/3 of the density
- Require Environmental Barrier Coatings (EBCs) for operation

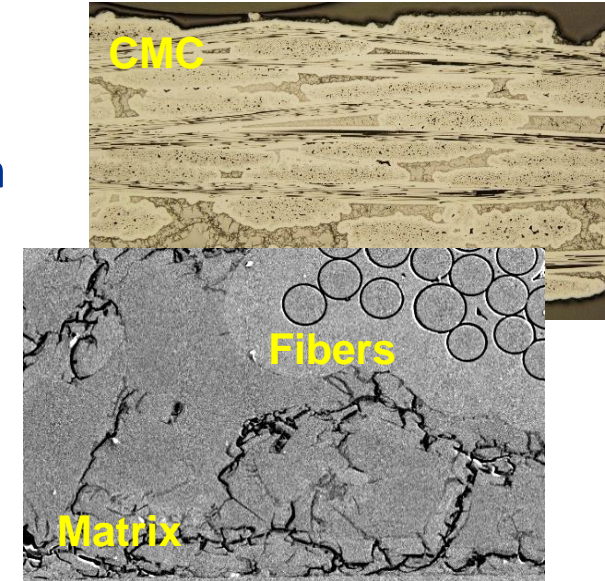
NASA is developing a material system with 2700°F capability

- This technology would reduce aircraft fuel burn by approximately an additional 6%, as well as lowering emissions

CMCs and EBCs

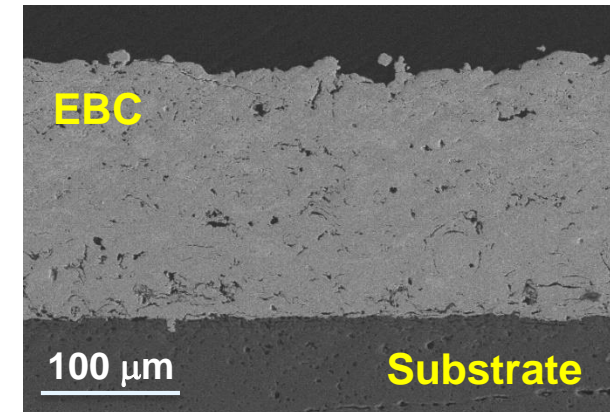
Ceramic Matrix Composites (CMCs)

- High temperature material of small diameter silicon carbide (SiC) fibers surrounded by a bulk SiC matrix
 - The matrix provides rigidity and overall shape
 - Fibers allow for crack deflection/toughness
 - React with water vapor in combustion environments



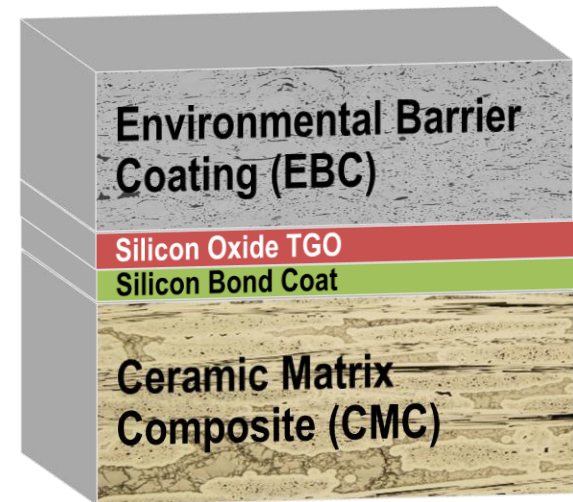
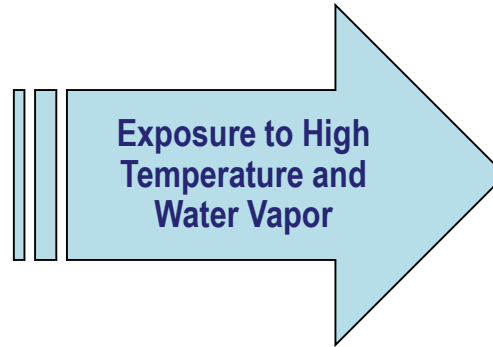
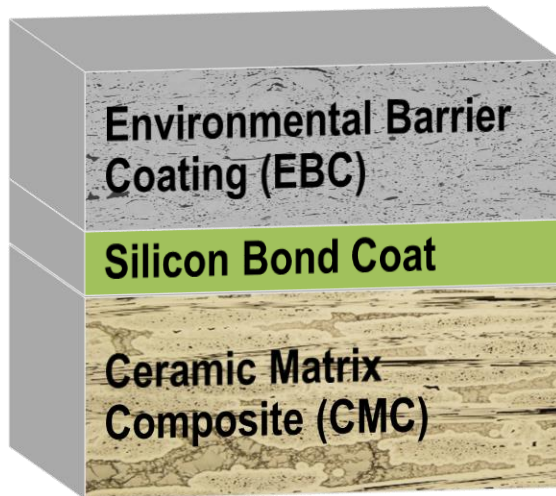
Environmental Barrier Coatings (EBCs)

- Needed to protect CMCs from engine environment
 - Can be single layer or multilayer
 - Typically oxides or silicates
 - Applied using a variety of methods

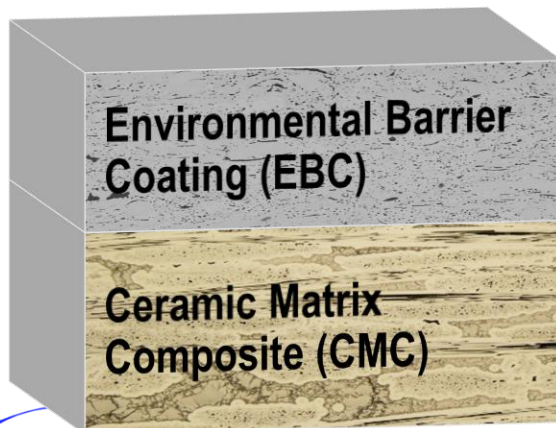


Environmental Barrier Coating (EBC) Systems

Low Temperature System (< 1316°C)



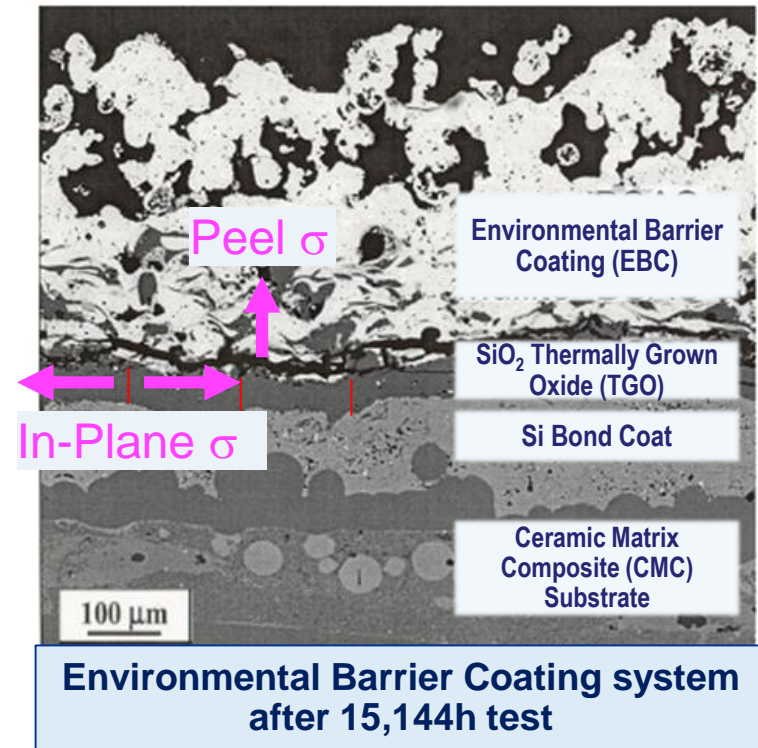
High Temperature System (> 1316°C)



**Thermally Grown Oxide (TGO)
is the Observed Point of Failure**

Environmental Barrier Coating (EBC) Systems

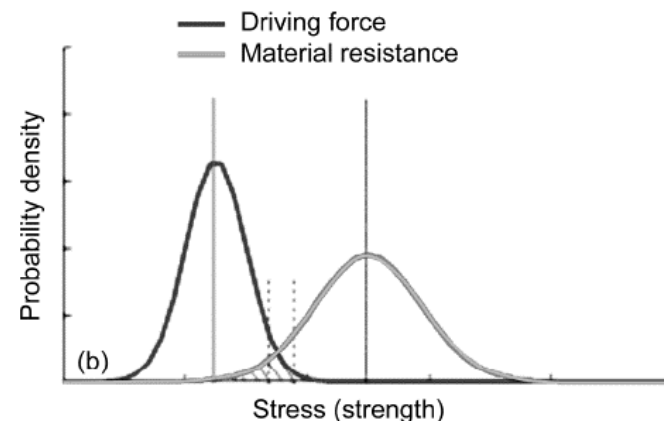
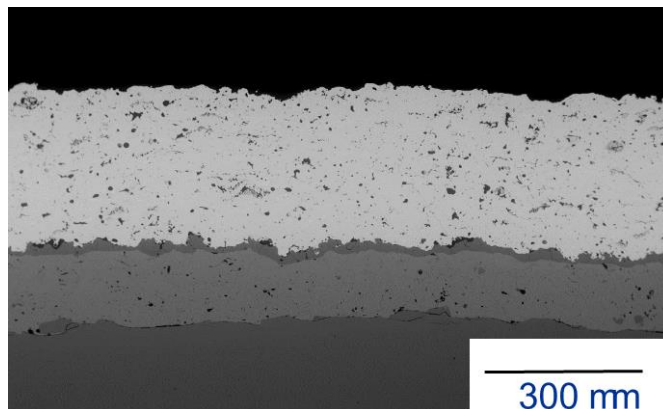
- Although durable, EBC systems must survive for 10,000+ hours
- Lifetime of EBC/CMC systems is limited by the formation of a thermally grown oxide (TGO)
 - SiO_2 TGO can grow on either silicon bond coat or SiC substrate
- Observed failures
 - Vertical Cracks
 - Horizontal Cracks (Delamination)
- Critical thickness for failure is roughly 20-30 microns
 - Can vary due to exposure temperature, microstructure, etc



Ultimate Goal: Predict the durability of EBC/CMC system when subjected to harsh environments

Current Study Objective

- Perform a *sensitivity study* to examine the influence of uniformly and nonuniformly grown oxide layers on the associated driving forces leading to mechanical failure (spallation) of EBC layer when subjected to isothermal loading
 - Ignore residual stresses due to processing
 - Ignore cyclic loading effects
 - **Qualitative** not quantitative study
 - Wanting to understand influence factors on driving forces away from the free edge
 - What influences critical TGO thickness
- Examined 3 layer and 4 layer system

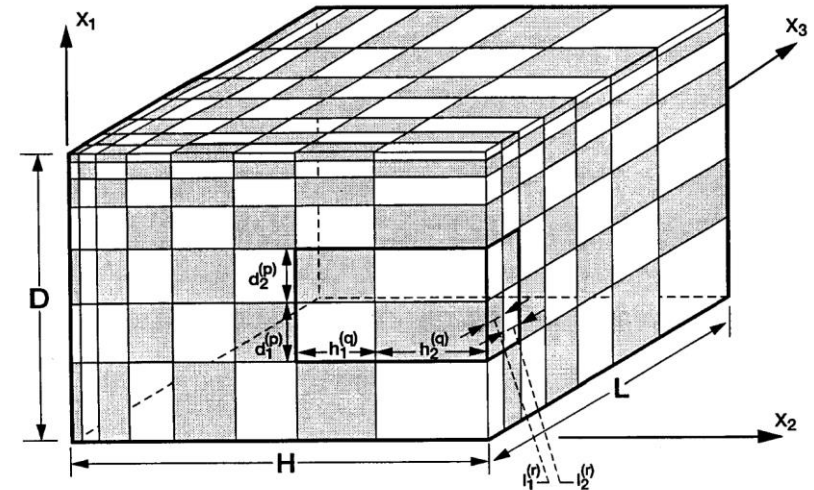


HOTFGM: High Order Theory for Functionally Graded Materials

HOTFGM offers a comprehensive approach towards analyzing/designing the response of components with various microstructural details.

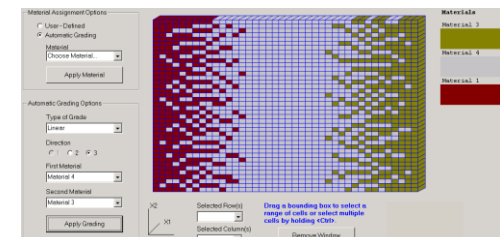
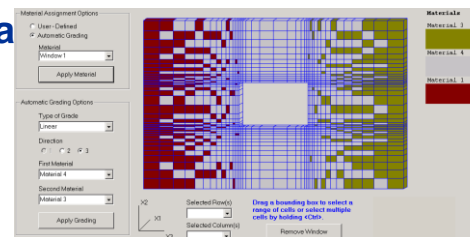
Capabilities include:

1. Combined thermal and mechanical analysis
2. Time-independent and time-dependent material behavior
3. Free-edge effects
4. Microstructure variability
5. Internal boundary cells (e.g. that can be used to represent internal cooling passages)
6. User-friendly graphical user interface
 - a. define material distribution with a variety of techniques for distributing materials
 - b. specify general thermal and mechanical boundary conditions,
 - c. view time dependent temperature, stress, and strain results.



2nd order Taylor Series Expansion of displacement

$$u_i^{(\alpha\beta\gamma)} = \bar{\epsilon}_{ij} x_j + W_{i(000)}^{(\alpha\beta\gamma)} + \bar{y}_1^{(\alpha)} W_{i(100)}^{(\alpha\beta\gamma)} + \bar{y}_2^{(\beta)} W_{i(010)}^{(\alpha\beta\gamma)} + \bar{y}_3^{(\gamma)} W_{i(001)}^{(\alpha\beta\gamma)} + \frac{1}{2} \left(3\bar{y}_1^{(\alpha)2} - \frac{d_\alpha^2}{4} \right) W_{i(200)}^{(\alpha\beta\gamma)} + \frac{1}{2} \left(3\bar{y}_2^{(\beta)2} - \frac{h_\beta^2}{4} \right) W_{i(020)}^{(\alpha\beta\gamma)} + \frac{1}{2} \left(3\bar{y}_3^{(\gamma)2} - \frac{l_\gamma^2}{4} \right) W_{i(002)}^{(\alpha\beta\gamma)}$$



*It has been commercialized by HyperSizer: Ncell

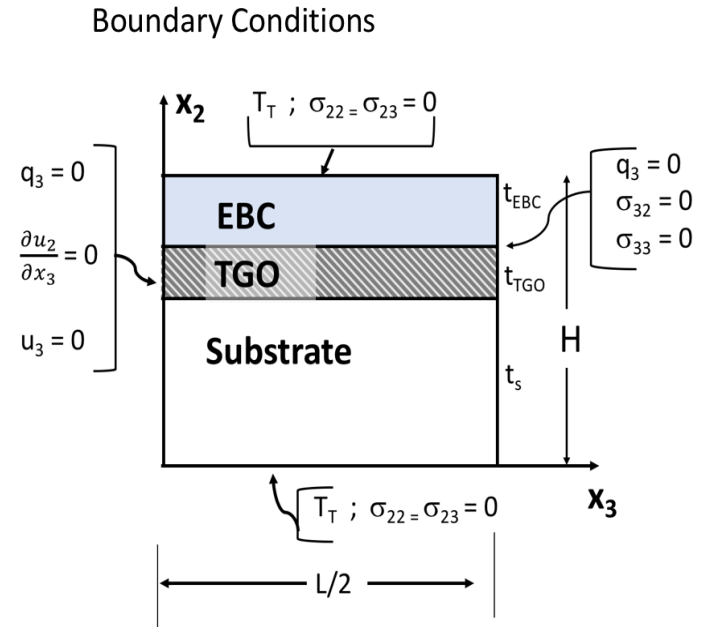
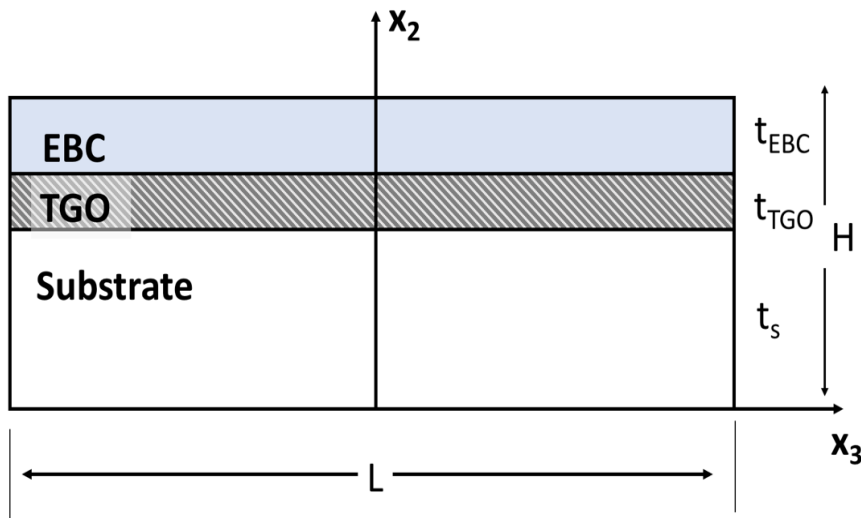
Constituents' Material Parameters

- Assume isotropic thermoelastic properties

Material	Thickness (mm)	Modulus (GPa)	Poisson Ratio	CTE ($\times 10^{-6} \text{ K}^{-1}$)	Conductivity (W/m-K)	Strength (MPa)
$\text{Yb}_2\text{Si}_2\text{O}_7$ (EBC)	0.175	200	0.27	4.5	1.25	45-65
SiO_2 (TGO)	0.001 0.002 0.004 0.008 0.016	35	0.17	10	1.4	45-75
Si (Bond Coat)	0.075	97	0.21	4.5	14.23	40-55
Hexoloy SiC (Substrate)	3.000*	400	0.17	5.25	30	380-550

* Initial thickness assuming no TGO, bond coat

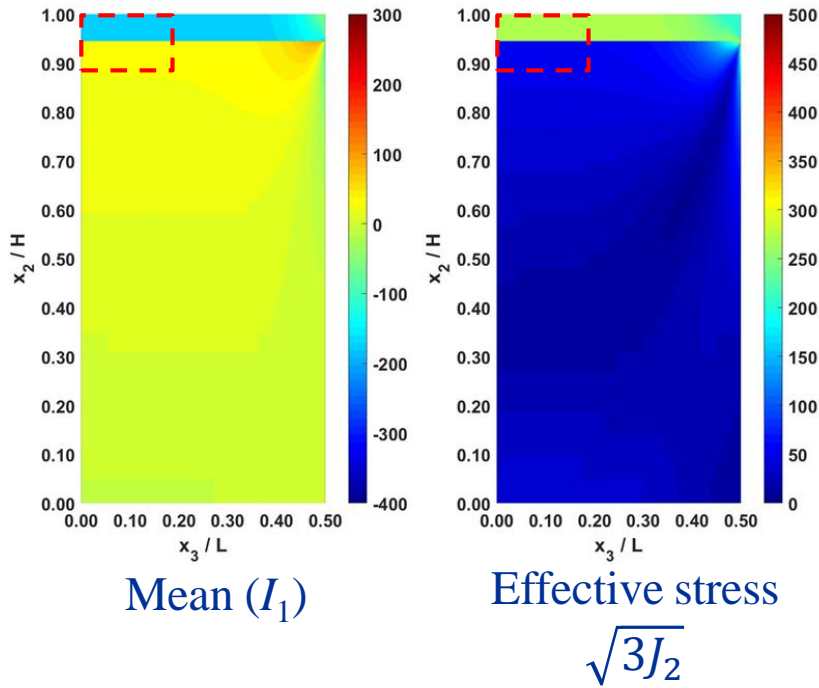
Idealization Of Three Layer System, With Geometry And Applied Thermal And Mechanical Boundary Conditions



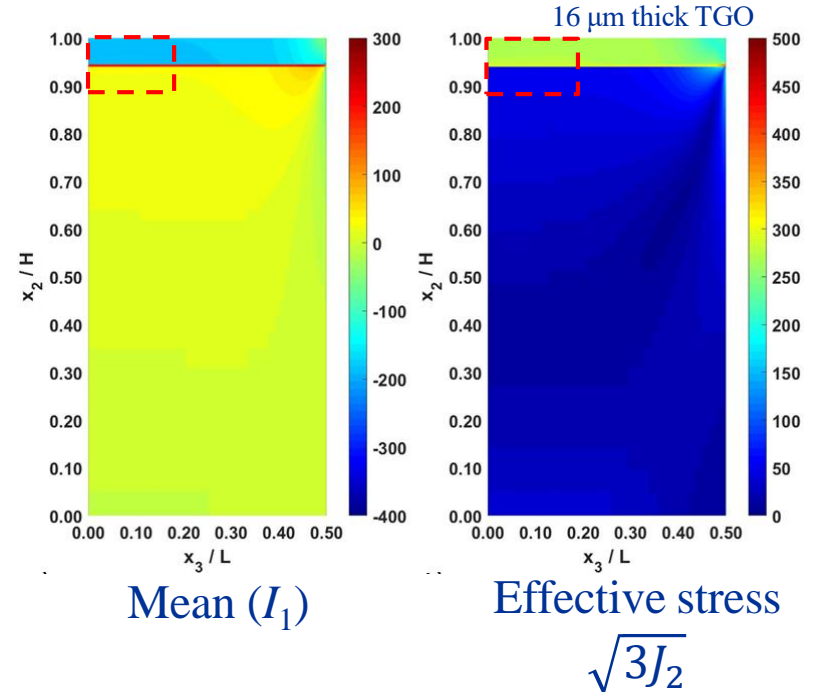
- Global loading is cool-down from 1482C to 38.7C (2700 °F to 102 °F)
- Applied in one step since material assumed to be linearly elastic
- Stress state is generated due to geometry and mismatch in constituent material properties

Results: Uniform Layers

Baseline: Two Layer (EBC/CMC)



Baseline: Three Layer (EBC/TGO/CMC)



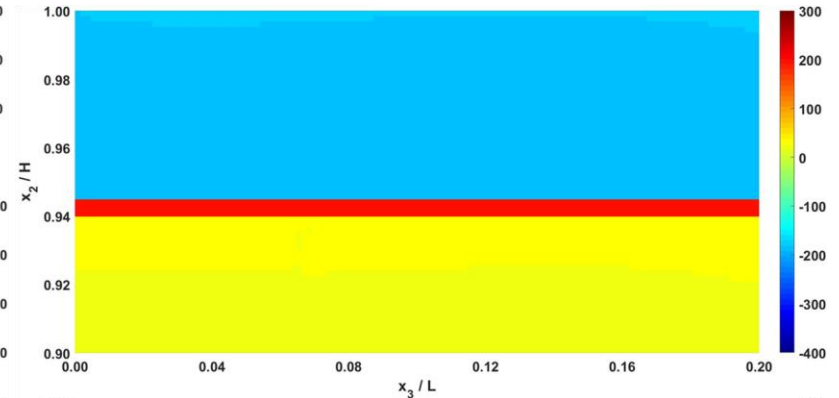
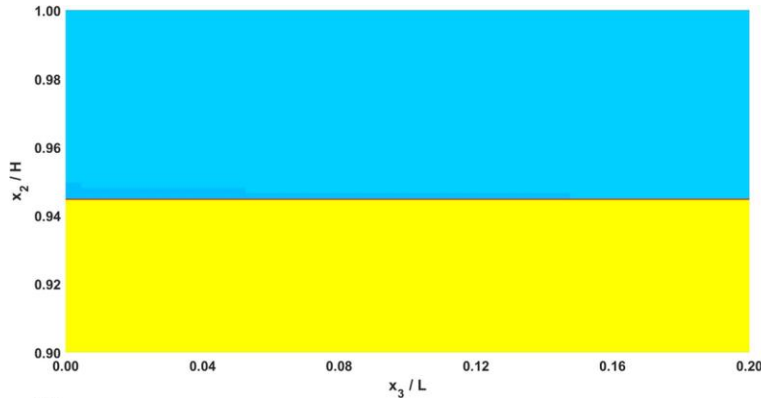
- Stress state uniform away from the free edge and throughout the TGO thickness

Results: Uniform Layers

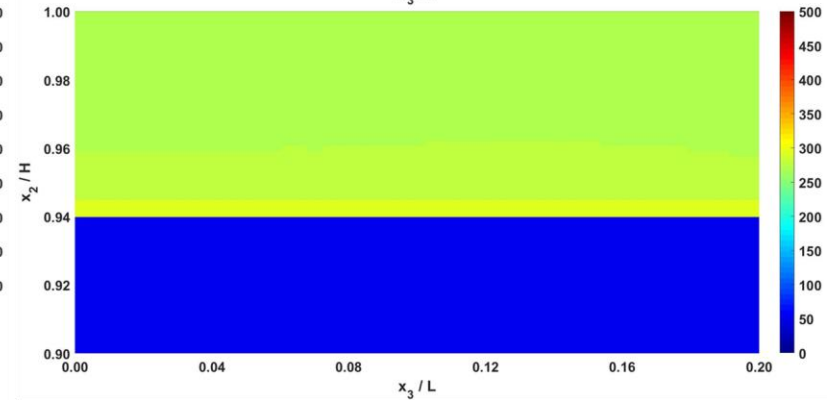
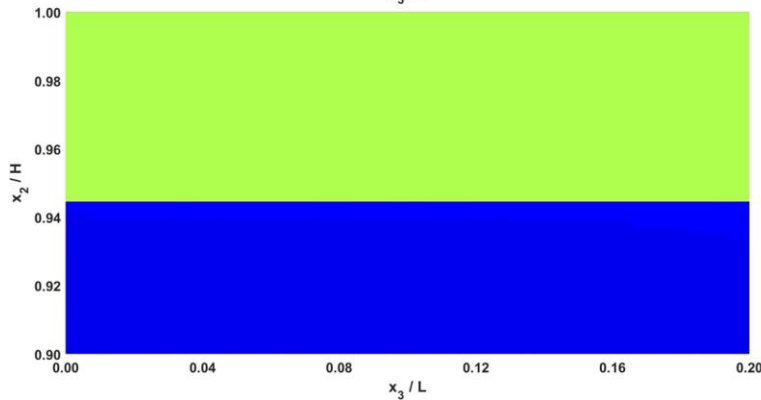
Thin 1 μm TGO Layer

Thick 16 μm TGO Layer

Mean Stress



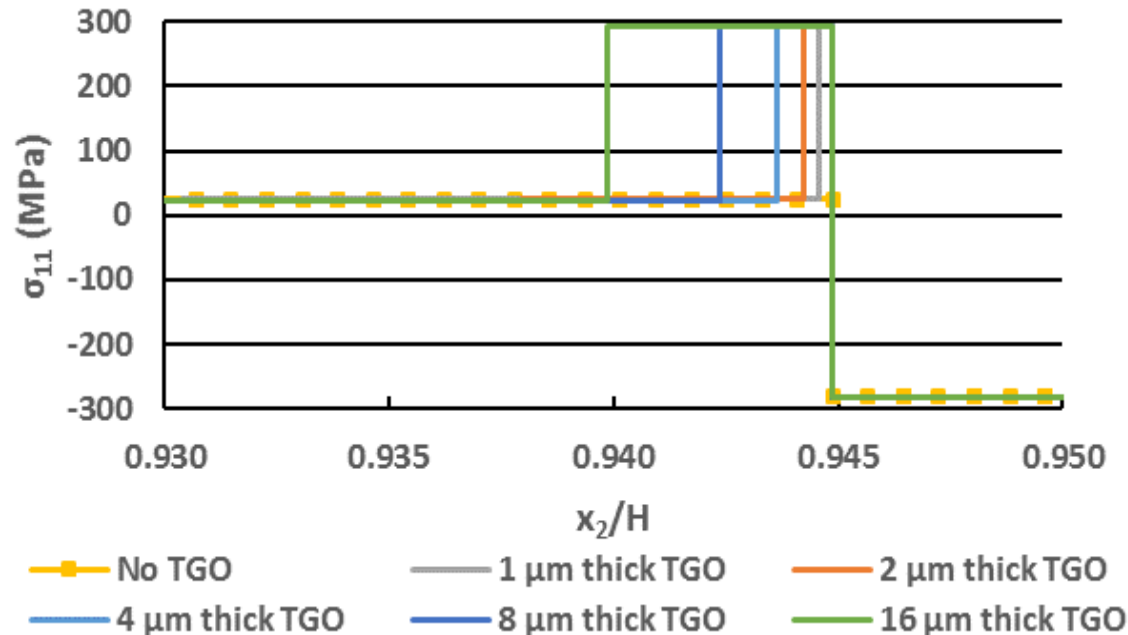
Effective Stress



- TGO thickness has no significant ($< 1\%$) effect on the resulting stress state in the system

Results: Uniform Layers

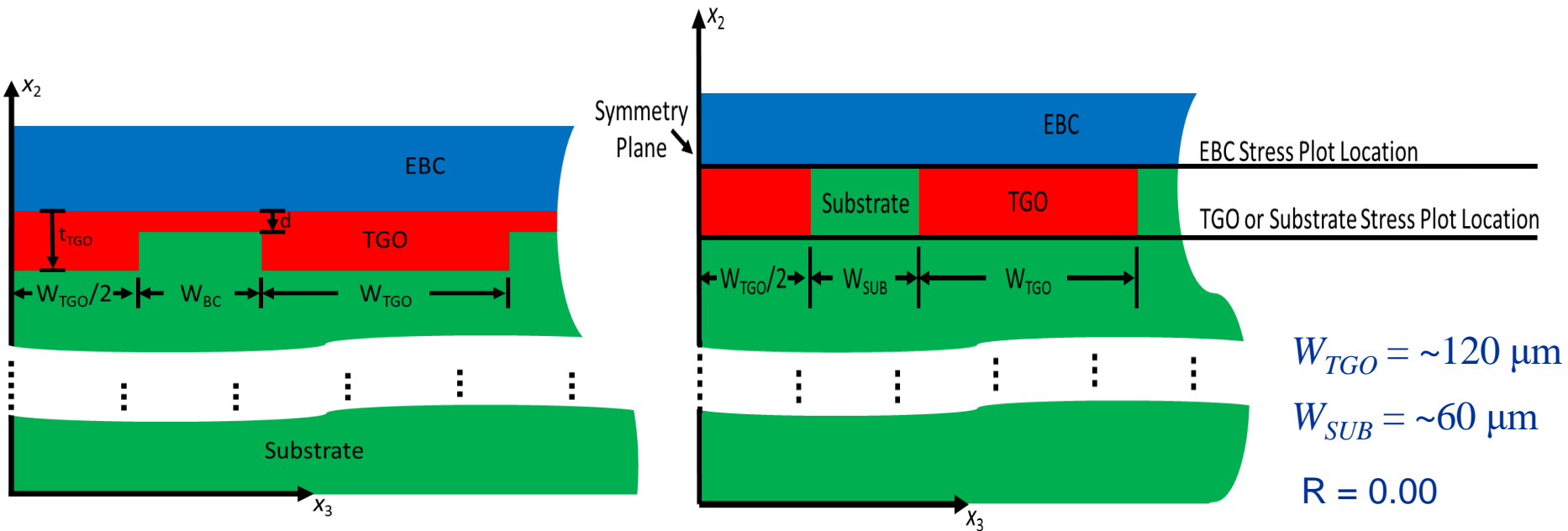
In-plane normal stress (σ_{11}) along the symmetry plane ($x_2 = 0$) near the substrate/TGO and TGO/EBC interfaces



- Magnitude of the tensile stress within the TGO remains nearly identical for all thickness (no criteria for calculating critical TGO thickness)
- Volume of TGO impacted by tensile stress however increases with thickness – thus suggesting that the resistance will most likely be reduced
- **In-plane stresses are only nonzero component – explains only vertical cracking**

Nonuniform Layer Idealization

Schematic showing discontinuous TGO layer geometry



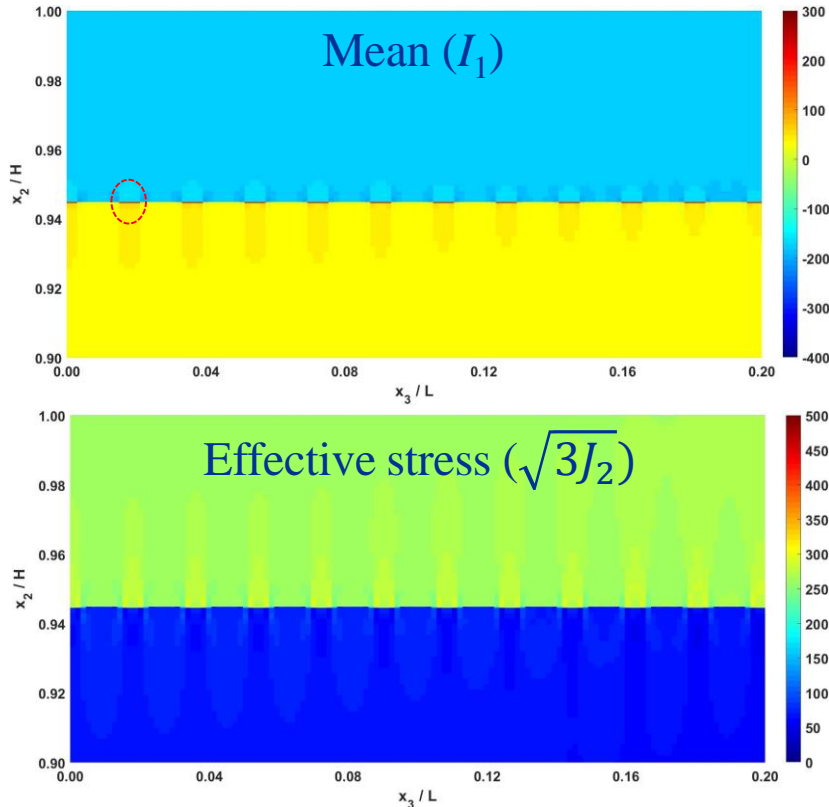
$$R = d/t_{TGO} \Rightarrow R = 0.00, 0.75, 1.00$$

$$t_{TGO} = 1, 4, 16 \mu m$$

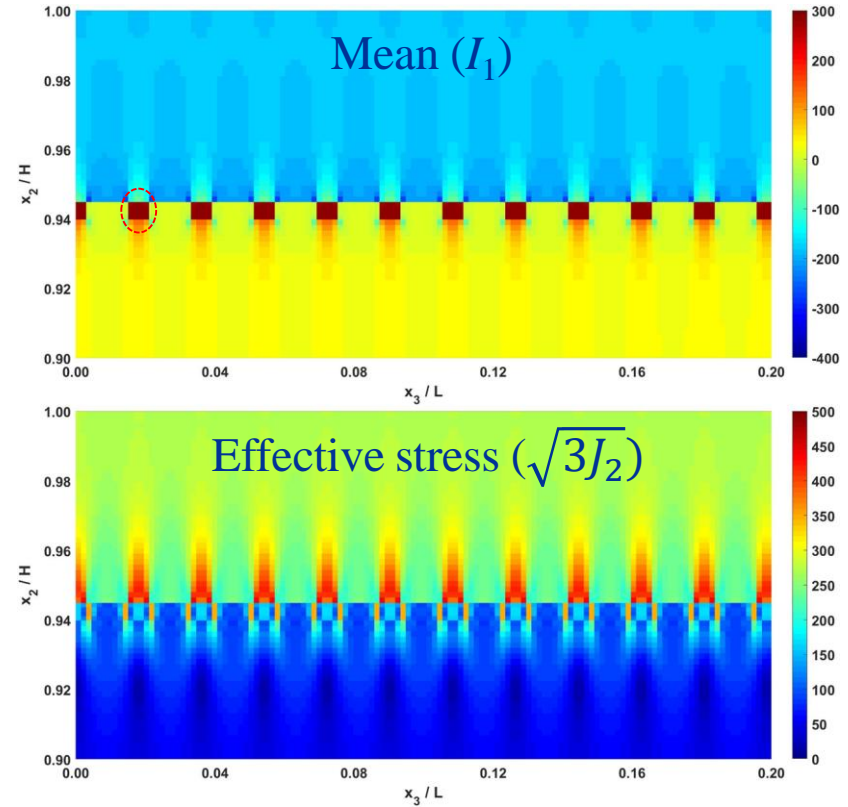
- EBC, TGO, and CMC substrate involving only the first $\sim 550 \mu m$ out of $5000 \mu m$ ($L/2$) in the x_3 -direction
- Discontinuous TGO “islands” inserted between the substrate and EBC interface
- Severity of nonuniformity considered by adjusting R factor
- Initial TGO island width was set to half its full width (symmetry boundary conditions)

Results: Nonuniform Layers

Thin 1 μm TGO Layer



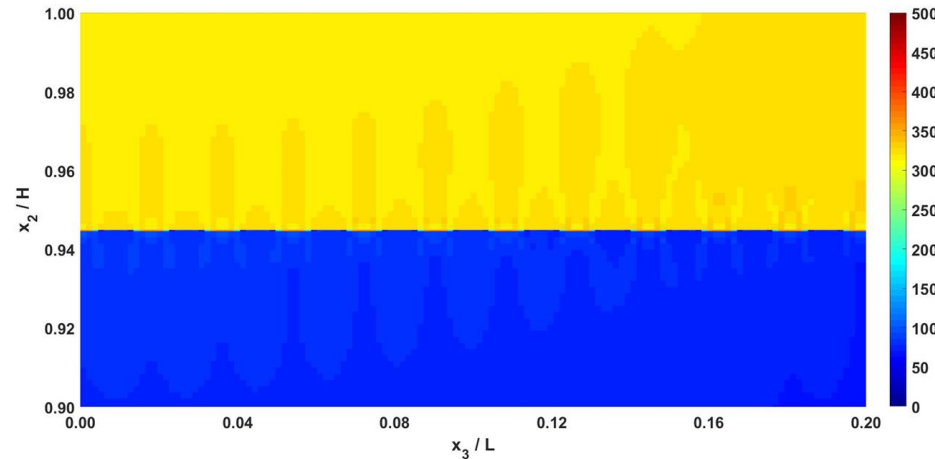
Thick 16 μm TGO Layer



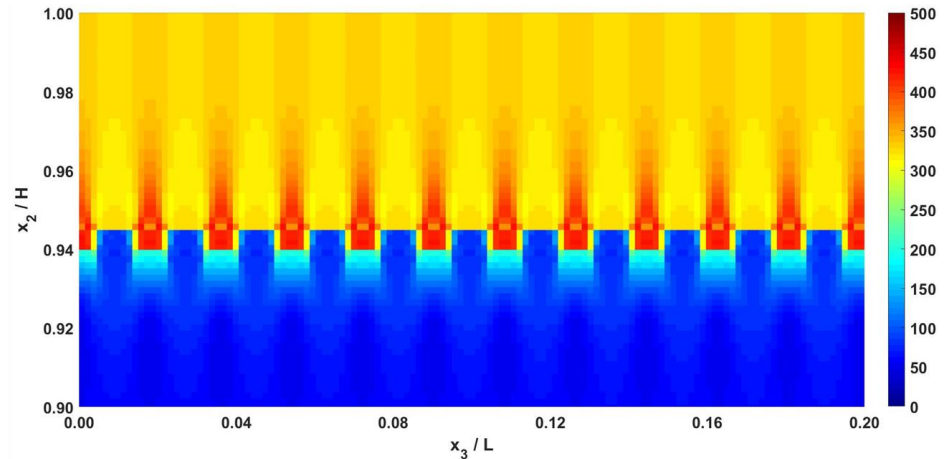
- Results are plotted away from free-edge
- Island edges introduce concentrations in both mean and effective stress
- As TGO thickness increases the magnitudes significantly increase

Results: Nonuniform Layers

Thin 1 μm TGO Layer



Thick 16 μm TGO Layer



- Equivalent damage stress from Lemaitre and Chaboche, Mechanics of solid materials
- Calculated by assuming equivalence in energy between multiaxial and uniaxial states

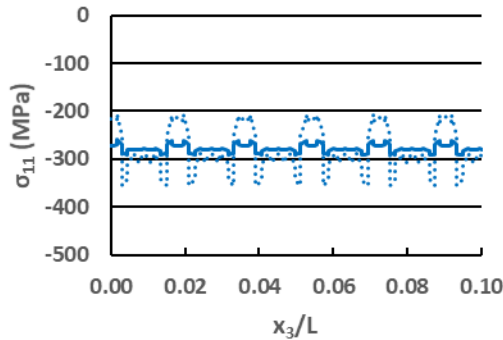
$$\sigma^* = \sigma_{eff} \sqrt{\frac{2}{3}(1 + \nu) + 3(1 - 2\nu) \left(\frac{\sigma_H}{\sigma_{eff}} \right)^2}$$

- Captures both mean and effective stress effects
- Increase in equivalent damage stress with increasing TGO thickness

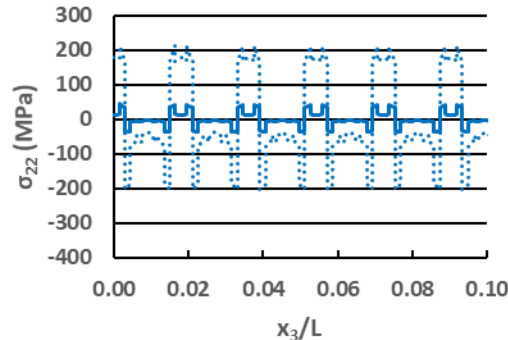
Nonuniformity in TGO Provides Driving Forces Consistent With EBC Spallation

EBC interface

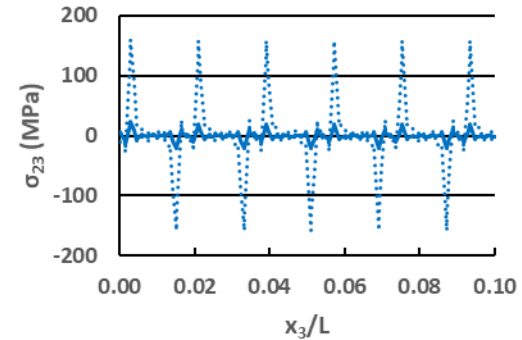
In-Plane Stress



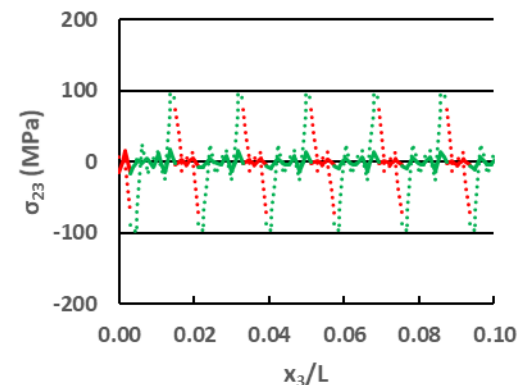
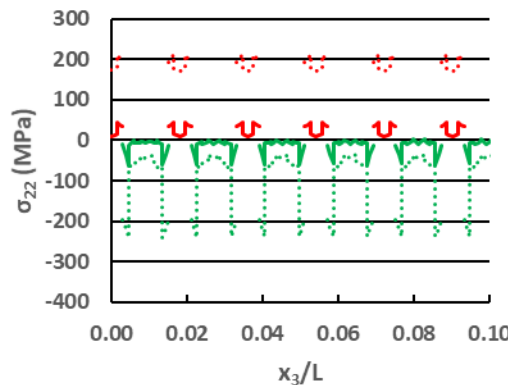
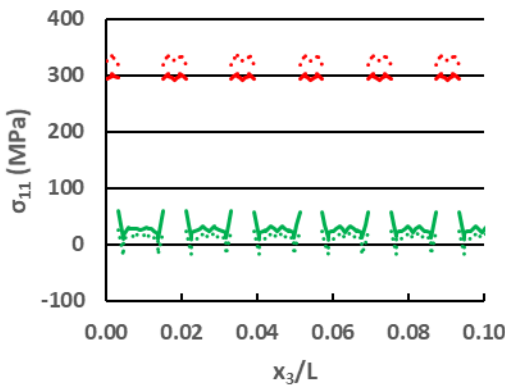
Peel Stress



Shear Stress



TGO or substrate interface

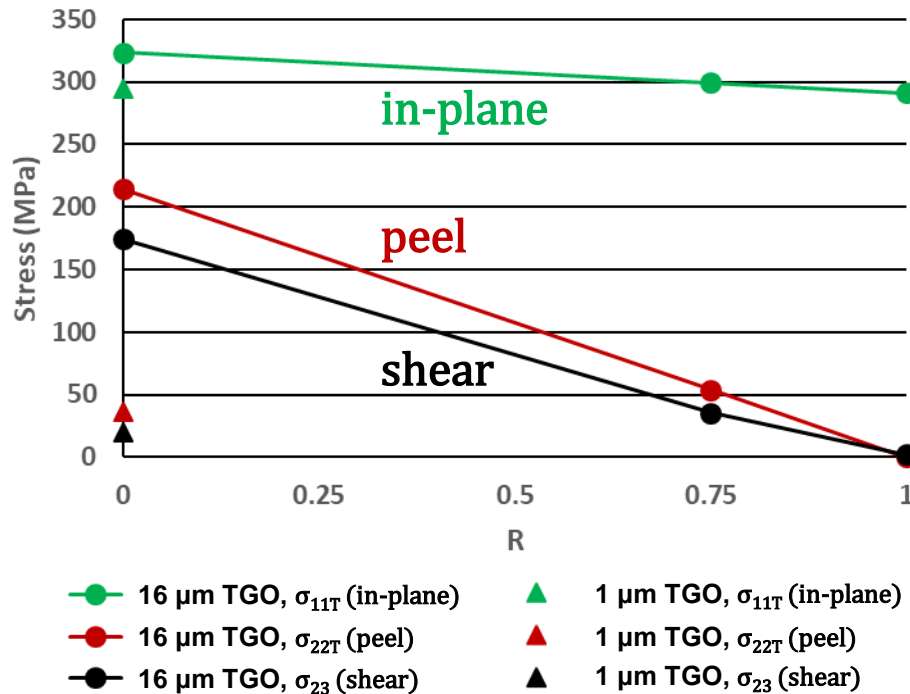


- High in-plane stress (σ_{11} , σ_{33}) – suggests vertical cracking likely
- Tensile peel stress (σ_{22}) – suggests potential EBC spallation in the vicinity of a TGO island
- High shear stress (σ_{23}) near boundaries – enhances likelihood for EBC spallation

Influence of Severity of Non-uniformity

$R = d/t_{TGO}$ \longrightarrow Lower value = more severe nonuniformity

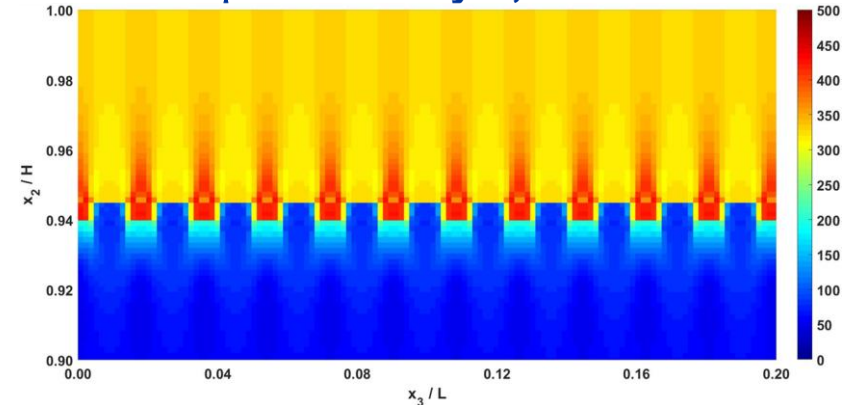
Max Stress vs. R factor



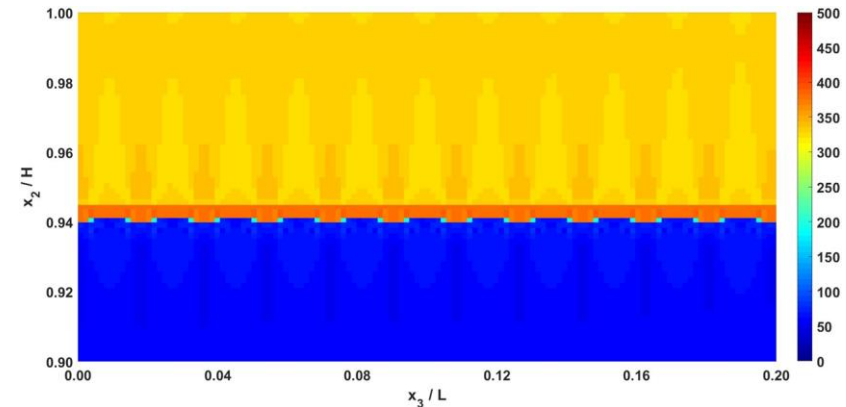
- As R increases, stresses decrease
 - reducing severity of nonuniformity = greater resistance to spallation
- Significant decrease in peel/shear stresses

Equivalent Damage Stress

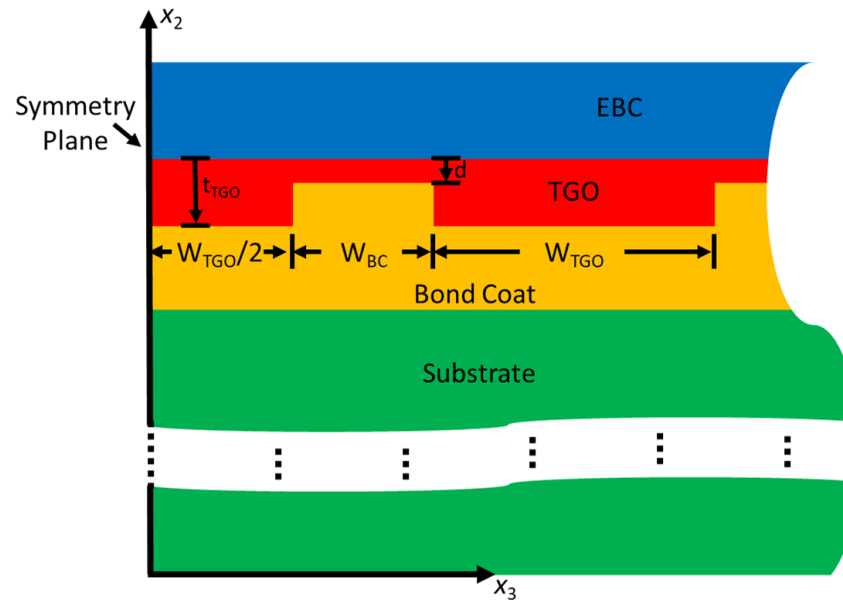
16 μm TGO Layer, R = 0.00



16 μm TGO Layer, R = 0.75



Nonuniform Idealization – 4 Layer System



$$t_{TGO} = 1, 4, 16 \mu\text{m} \quad R = d/t_{TGO}$$

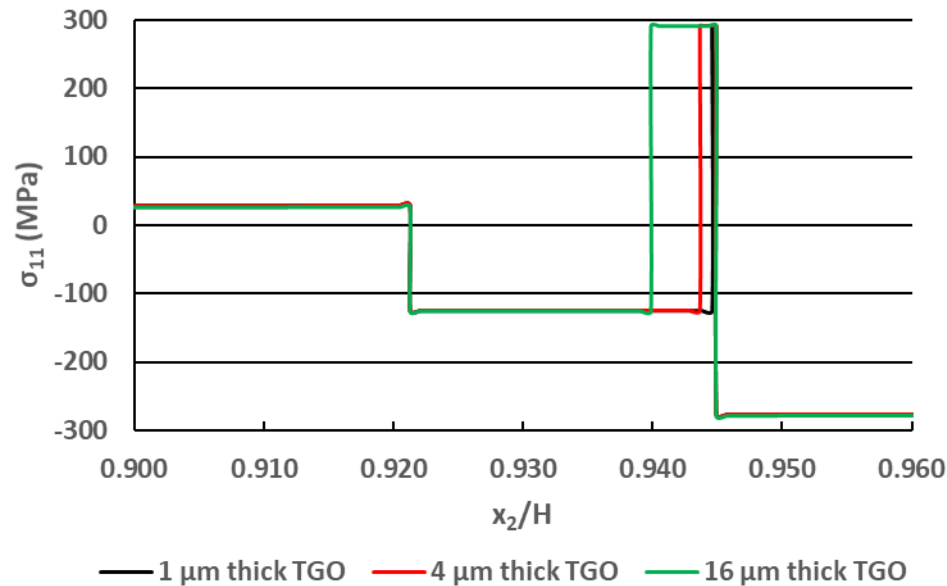
$$W_{TGO} = \sim 120 \mu\text{m} \quad R = 0.00, 1.00$$

$$W_{BC} = \sim 60 \mu\text{m}$$

- Discontinuous TGO “islands” inserted between the substrate and EBC interface
- Severity of nonuniformity considered by adjusting R factor

Uniform TGO – 4 Layer System

In-plane normal stress (σ_{11}) along the symmetry plane ($x_2 = 0$) near the substrate/bond coat, bond coat/TGO, and TGO/EBC interfaces

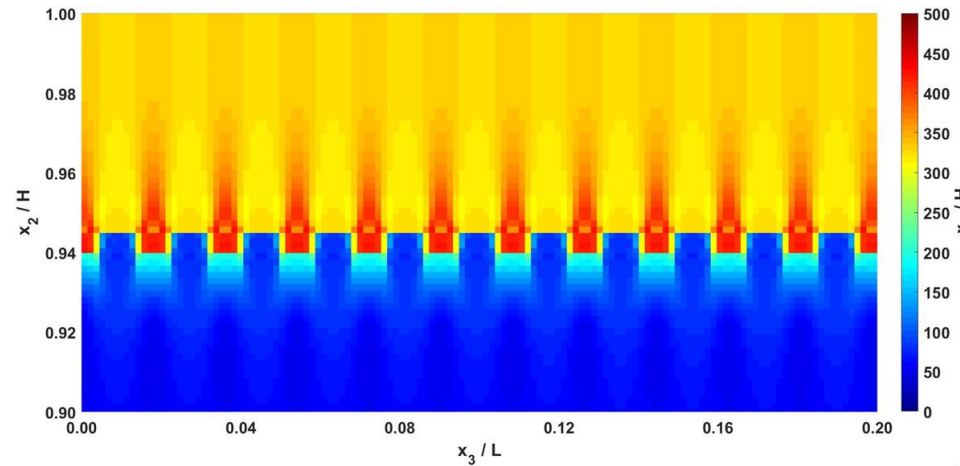


- Stress state insensitive to TGO thickness – similar to 3 layer system results
- Suggest no cracking in Si-bond coat due to compressive stress state

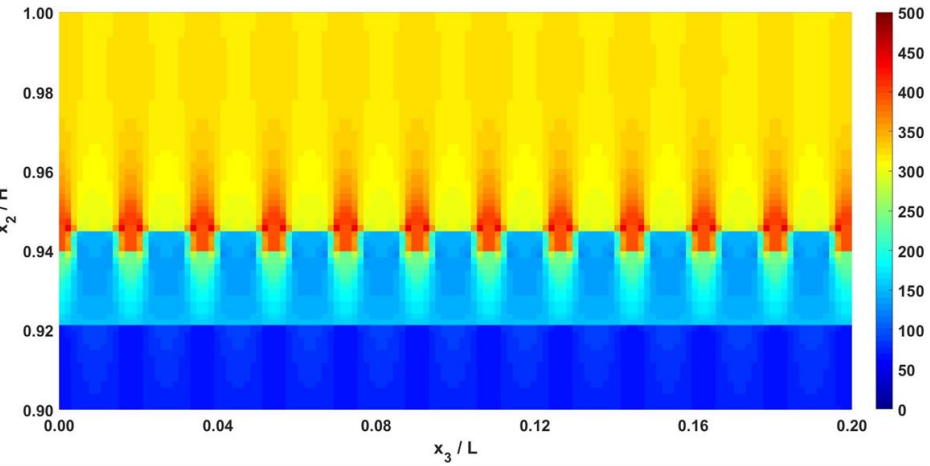
Presence of Si Bond Coat Reduces Equivalent Damage Stress

Equivalent Damage Stress - 16 μm TGO Layer, $R = 0.00$

3 Layer System

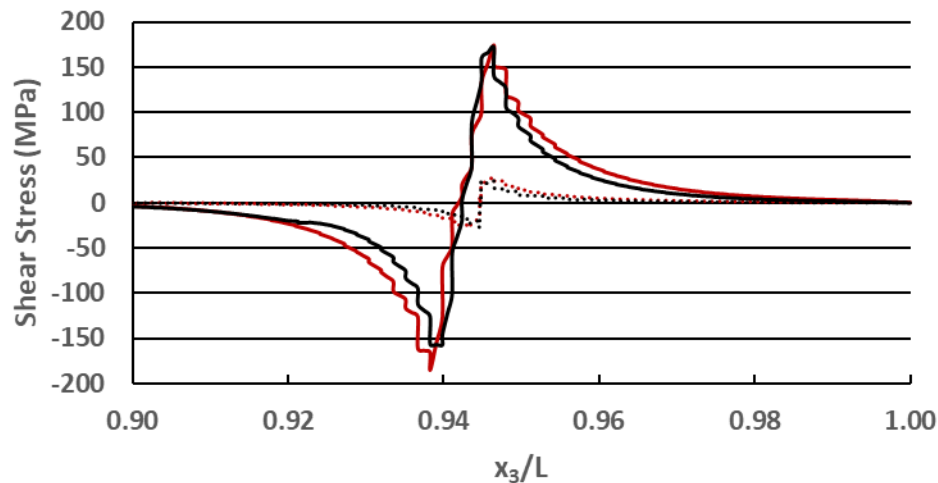
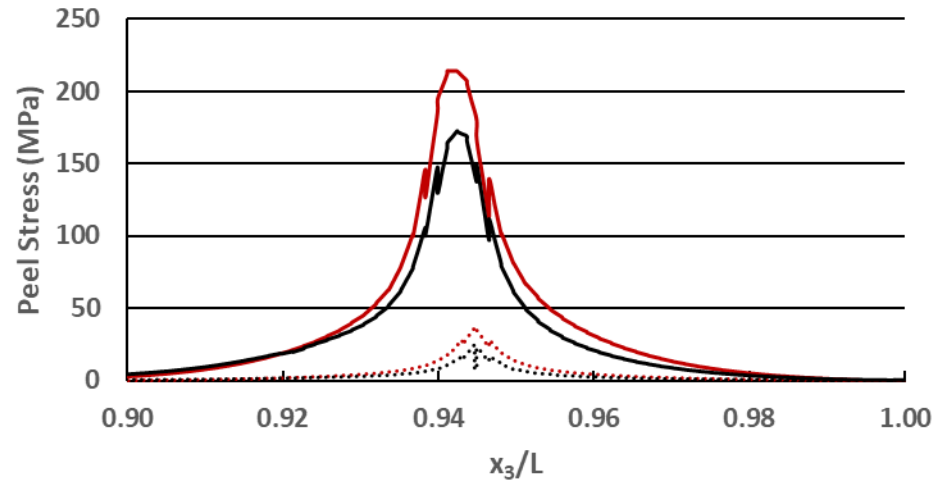


4 Layer System

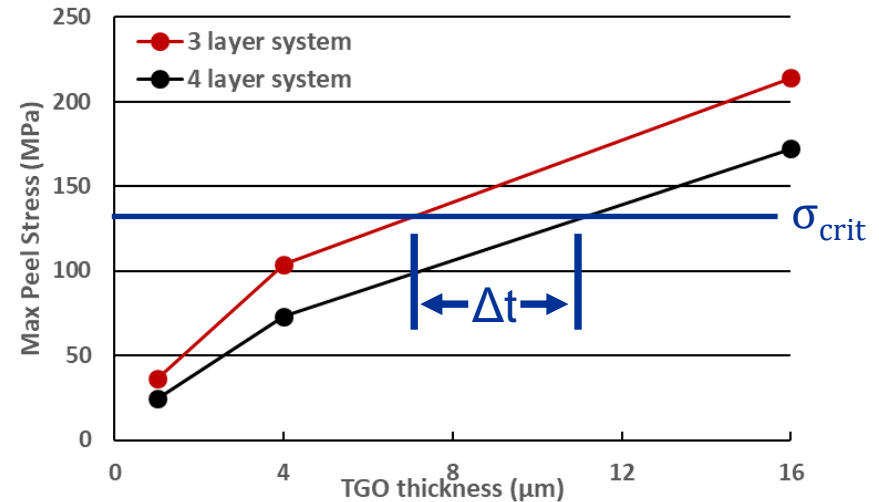


- Lower stress in TGO for 4 layer system

Presence of Si Bond Coat Reduces Driving Forces



..... 3 layer - 1 μm thick TGO
 4 layer - 1 μm thick TGO
 — 3 layer - 16 μm thick TGO
 — 4 layer - 16 μm thick TGO



- Decrease in peel stress when bond coat added
- Shear stresses similar
- **Given critical failure stress, Si bond coat (i.e., four layer system) enables thicker TGO layer prior to failure**

Conclusions

- HOTFGM tool enables efficient study of microstructural features (e.g., volume fraction, geometry, constituent phases, etc.) on overall composite response.

Uniform TGO layers

- Stress state is constant away from free-edge.
- TGO thickness had a negligible effect on the magnitude of the stress state.
- To determine critical TGO thickness, change in material resistance must be included.

Nonuniform TGO layers

- Significant peel and shear stresses were predicted to occur in both the TGO and EBC near these non-uniformities.
 - Magnitude of these components influenced based on thickness of TGO and severity of non-uniformity.
 - These stresses could explain the onset and evolution of TGO damage and ultimately EBC spallation when a critical TGO thickness is reached.
- The idealized model considered in this study represents a first step at understanding the influence of TGO geometric nonuniformity on the stress state in a CMC/EBC system.

Future Work

material behavior (anisotropic, creep, damage, TGO evolution)
thermomechanical cycling

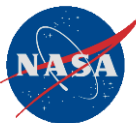
Thank You For Your Attention



Email: Trenton.M.Ricks@nasa.gov



Glenn Research Center at Lewis Field

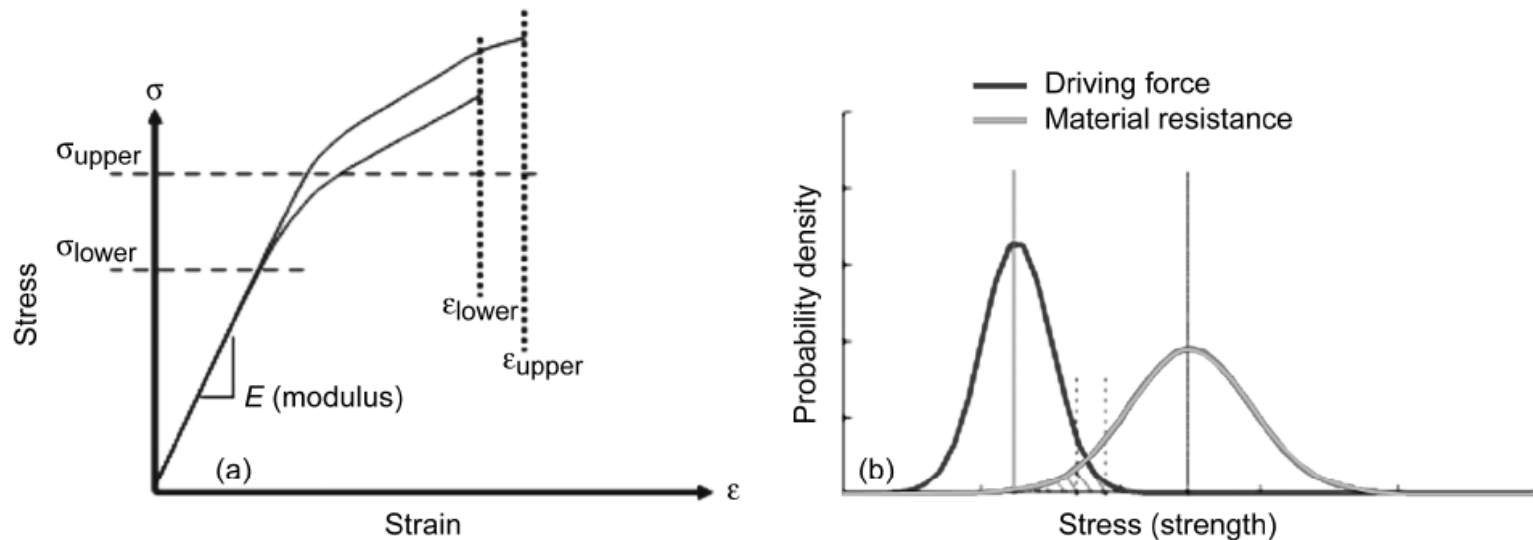


Prior Study Results related to Thermally Induced Stresses in TBC-Protected Plate

- Effect of **geometry** on free-edge interlaminar stresses: no effect of L/H, significant effect of t_{BC}/H
- Effect of **bond coat** properties on free-edge interlaminar stresses: significant effect of α_{BC} and E_{BC} , small effect of κ_{BC}
- Effect of **top coat** properties on free-edge interlaminar stresses: smaller effect of α_{TC} and E_{TC} relative to α_{BC} and E_{BC}
- Effect of **substrate** properties on free-edge interlaminar stresses: relatively small effect of α_s and E_s along TC/BC interface, with substantially greater effect along BC/S interface
- Effect of **through-thickness thermal gradient** on free-edge interlaminar stresses: the magnitude of the gradient has significant effect
 - Change in sign of the peel stress with increasing gradient from tension to compression

* “Thermally-Induced Interlaminar stresses in TBC-Protected Plate: A Material and Geometric Parametric Study”; Arnold et al., HITEMP Review 1995, Vol. II, CP 10178, pp. 34:1-14

Modeling Philosophy: Trade Offs



Actuality both driving force (applied loads and local architecture) and material resistance (dependent upon both local architecture and processing methodology) are spatially varying throughout a given component/specimen.

- 1) Assume a fixed (pristine) architecture (**Driving Forces**) with specific architectural parameters that can be varied (e.g., tow spacing, tow shape, etc.) to obtain a statistical distribution of resulting stresses. These stresses then can be compared with statically and spatially varying material strength values (**Resistance**).
- 2) Alternatively, one can analyze local architecture (e.g., ply shifting, ply rotation, nesting, etc.) and the flaw and porosity distribution in great detail using high-fidelity numerical analyses to obtain detailed local stresses (i.e., **driving forces**). These stresses can be compared with a fixed value of material strength (**resistance**).